Biopolymers

Contents

Volume 33, 1993

Issue 1, January 1993

Solution Structure of Peptides Containing Two Dehydro-Phenylalanine Residues: A CD Investigation / 1
O. Pieroni, A. Fissi, C. Pratesi, P. A. Temussi, and F. Ciardelli

Hydrational and Intrinsic Compressibilities of Globular Proteins / 11
D. P. Kharakoz and A. P. Sarvazyan

NMR Studies of an Extrahelical Cytosine in an A·T Rich Region of a Deoxyribodecanucleotide / 27
K. M. Morden and K. Maskos

Influence of Electrostatic Interactions on the Sugar–Phosphate Backbone Conformation in DNA / 37
V. I. Pechenaya

Measurement of Restricted Rotational Diffusion of Fluorescent Lipids in Supported Planar Phospholipid Monolayers Using Angle-Dependent Polarized Fluorescence Photobleaching Recovery / 45
M. M. Timbs and N. L. Thompson

Calculation and Measurement of the Dipole Moment of Small Proteins: Use of Protein Data Base / 59
S. Takashima and K. Asami

Degree of Linear Polarization Method for Determination of Intrinsic Optical Anisotropy of Southern Bean Mosaic Virus / 69
Y. Sano

A Monte Carlo Method for Generating Structures of Short Single-Stranded DNA Sequences / 75
D. A. Erie, K. J. Breslauer, and W. K. Olson

Application of Distance Geometry to the Proton Assignment Problem / 107
C. M. Oshiro and I. D. Kuntz

Volume Changes Correlate with Entropies and Enthalpies in the Formation of Nucleic Acid Homoduplexes: Differential Hydration of A and B Conformations / 117
D. Rentzeperis, D. W. Kupke, and L. A. Marky

Kinetic Analysis of the Hydrodynamic Transition Accompanying Protein Folding Using Size Exclusion Chromatography. 1. Denaturant Dependent Baseline Changes / 127
W. Shalongo, P. Heid, and E. Stellwagen

Kinetic Analysis of the Hydrodynamic Transition Accompanying Protein Folding Using Size Exclusion Chromatography. 2. Comparison of Spectral and Chromatographic Kinetic Analyses / 135
W. Shalongo, M. Jagannadham, and E. Stellwagen

Microwave Absorption Spectroscopy of DNA / 147
I. J. Bigio, T. R. Gosnell, P. Mukherjee, and J. D. Saffer

Temperature-Induced Conformational Transition in Xanthans with Partially Hydrolyzed Side Chains / 151
B. E. Christensen, K. D. Knudsen, O. Smidsrød, S. Kitamura, and K. Takeo

Helix-Forming Tendencies of Amino Acids Depend on Their Sequence Contexts: Tripeptides AFG and FAG Show Incipient β-Bulge Formation in Their Crystal Structures / 163
R. Parthasarathy, K. Go, and S. Chaturvedi

Necessary Conditions for Avoiding Incorrect Polypeptide Folds in Conformational Search by Energy Minimization / 173
S. Vajda, M. S. Jafri, O. U. Sezerman, and C. DeLisi

RESEARCH COMMUNICATION

Macromolecular Cyclization of (1 → 6)-Branched-(1 → 3)-β-D-Glucans Observed After Denaturation–Renaturation of the Triple-Helical Structure / 193
B. T. Stokke, A. Elgsaeter, D. A. Brant, T. Kuge, and S. Kitamura

ERRATUM

Conformation of Uteroglobin Fragments / 199
S. Mammi, M. T. Foffani, S. Improta, M. Tessari, E. Schievano, and E. Peggion

Issue 2, February 1993

Characterization of β-Turns in Cyclic Hexapeptides in Solution by Fourier Transform IR Spectroscopy / 201
H. H. Mantsch, A. Perczel, M. Hollósi, and G. D. Fasman

Peptide Design 3_{10}-Helical Conformation of a Linear Pentapeptide Containing Two Dehydrophenylalanines, Boc-Gly-Δ^ZPhe-Leu-Δ^ZPhe-Ala-$NHCH_3$ / 209
K. K. Bhandary and V. S. Chauhan

Approximation and Characterization of Molecular Surfaces / 219
B. S. Duncan and A. L. Olson

Shape Analysis of Molecular Surfaces / 231
B. S. Duncan and A. J. Olson

Photodynamic Induction of DNA–Protein Cross-Linking in Solution by Several Sensitizers and Visible Light / 239
A. Villanueva, M. Cañete, C. Trigueros, L. Rodriguez-Borlado, and A. Juarranz

Linear Dichroism Demonstrates that the Bases in Poly[d(AC)] · Poly[d(GT)] and Poly-[d(AG)] · Poly[d(CT)] Are Inclined from Perpendicular to the Helix Axis / 245
H. Kang and W. C. Johnson, Jr.

Conformational Preference Functions for Predicting Helices in Membrane Proteins / 255
D. Juretić, B. Lee, N. Trinajstić and R. W. Williams

Crystal Structure, Conformational Analysis, and Molecular Dynamics of Tetra-*O*-Methyl-(+)-Catechin / 275
F. R. Fronczek, R. W. Hemingway, G. W. McGraw, J. P. Steynberg, C. A. Helfer, and W. L. Mattice

X-Ray Studies on Crystalline Complexes Involving Amino Acids and Peptides. XXIV. Different Ionization States and Novel Aggregation Patterns in the Complexes of Succinic Acid with DL- and L-Histidine / 283
G. S. Prasad and M. Vijayan

Predicting Polypeptide and Protein Structures from Amino Acid Sequence: Antlion Method Applied to Melittin / 293
T. Head-Gordon and F. H. Stillinger

Permethylation Alters the Conformational Transitions and the Complexing Ability of Melittin: A Model for Methylated Proteins / 305
K. Ramalingam, J. Bello, and S. Aimoto

Vibrational CD Study of the Thermal Denaturation of Poly(rA)·Poly(rU) / 315
L. Yang and T. A. Keiderling

Announcement / 328

Issue 3, March 1993

Exhaustive Conformational Search and Simulated Annealing for Models of Lattice Peptides / 329
R. C. Brower, G. Vasmatzis, M. Silverman, and C. Delisi

Persistence Analysis of the Static and Dynamical Helix Deformations of DNA Oligonucleotides: Application to the Crystal Structure and Molecular Dynamics Simulation of d(CGCGAATTCGCG)$_2$ / 335
C. Prévost, S. Louise-May, G. Ravishanker, R. Lavery, and D. L. Beveridge

A Cooperative Self-Consistent Microscopic Theory of Thermally Induced Melting of a Repeat Sequence DNA Poylmer / 351
Y. Z. Chen and E. W. Prohofsky

The Structure of the Left-Handed Antiparallel Amylose Double Helix: Theoretical Studies / 363
W. Schulz, H. Sklenar, W. Hinrichs, and W. Saenger

A Model for the Dynemicin-A Cleavage of DNA Using Molecular Dynamics Simulation / 377
M. G. Cardozo and A. J. Hopfinger

Synthetic Peptide and Template-Assembled Synthetic Protein Models of the Hen Egg White Lysozyme 87–97 Helix: Importance of a Protein-Like Framework for Conformational Stability in a Short Peptide Sequence / 389
S. Vuilleumier and M. Mutter

Accomodation of a D-Phe Residue into a Right-Handed 3_{10}-Helix: Structure of Boc-D-Phe-(Aib)$_4$-Gly-L-Leu-(Aib)$_2$-OMe, an Analogue of the Amino Terminal Segment of Antiamoebins and Emerimicins / 401
I. L. Karle, J. L. Flippen-Anderson, K. Uma, and P. Balaram

Hydrodynamic Modes of Arbitrarily Shaped Flexible Macromolecules: Influence on Dynamic Light Scattering / 409
R. F. Goldstein

Synthesis, Conformation, and Activity of HCO-Met-Δ^zLeu-Phe-OMe, an Active Analogue of Chemotactic *N*-Formyltripeptides / 437
G. P. Zecchini, M. P. Paradisi, I. Torrini, G. Lucente, E. Gavuzzo, F. Mazza, G. Pochetti, M. Paci, M. Sette, A. Di Nola, G. Veglia, S. Traniello, and S. Spisani

The Preparation and Characterization of a Twin-Tailed, Lipid-Linked Polysialic Acid / 453
I. Matthews and K. Petrak

Molecular Dynamics Simulations of B-DNA: An Analysis of the Role of Initial Molecular Configuration, Randomly Assigned Velocity Distribution, Long Integration Times, and Nonconstrained Termini / 459
S. Falsafi and N. O. Reich

Calcium-Dependence of Laminin Binding to Phospholipid Membranes / 475
J. J. Ramsden

Looking into the Grooves of DNA / 479
N. Boutonnet, X. Hui, and K. Zakrzewska

Helix Promotion in Polypeptides by Polyols / 491
J. Bello

Ca^{2+}-Induced Conformational Transitions of Phosphorylated Peptides / 497
M. Hollósi, L. Ötvös, Jr., L. Ürge, J. Kajtár, A. Perczel, I. Laczkó, Z. Vadász, and G. D. Fasman

Announcement / 511

Issue 4, April 1993

The Influence of Hydration on the Conformation of Lysozyme Studied by Solid-State ^{13}C-NMR Spectroscopy / 513
R. B. Gregory, M. Gangoda, R. K. Gilpin, and W. Su

Effects of Molecular Association on Structure and Dynamics of a Collagenous Peptide / 521
V. A. Daragan, E. Ilyina, and K. H. Mayo

^{1}H, ^{13}C, and ^{15}N Assignments and Secondary Structure of the FK506 Binding Protein When Bound to Ascomycin / 535
R. X. Xu, D. Nettesheim, E. T. Olejniczak, R. Meadows, G. Gemmecker, and S. W. Fesik

Dynamic Light Scattering of Aqueous Solutions of Linear Aggregates Induced by Thermal Denaturation of Ovalbumin / 551
N. Nemoto, A. Koike, K. Osaki, T. Koseki, and E. Doi

Physicochemical Properties of (1 → 6)-Branched (1 → 3)-β-D-Glucans. 1. Physical Dimensions Estimated from Hydrodynamic and Electron Microscopic Data / 561
B. T. Stokke, A. Elgsaeter, C. Hara, S. Kitamura, and K. Takeo

Molecular Dynamics Study of Iduronate Ring Conformation / 575
M. J. Forster and B. Mulloy

Reversible Effects of Medium Dielectric Constant on Structural Transformation of β-Lactoglobulin and Its Retinol Binding / 589
E. Dufour, C. Bertrand-Harb, and T. Haertlé

Diagonalization in a Mixed Basis: A Method to Compute Low-Frequency Normal Modes for Large Macromolecules / 599
L. Mouawad and D. Perahia

Design of Peptides: Crystal and Molecular Structure of a 3_{10}-Helical Peptide N-Boc-L-Phe-dehydro-Phe-L-Val-L-Phe-dehydro-Phe-L-Val-OCH_3 / 613
B. Padmanabhan and T. P. Singh

β-Alanine Containing Peptides: γ-Turns in Cyclotetrapeptides / 621
B. Di Blasio, A. Lombardi, G. DAuria, M. Saviano, C. Isernia, O. Maglio, L. Paolillo, C. Pedone, and V. Pavone

Rayleigh Scattering of Mössbauer Radiation in Hydrated Oriented DNA Fibers / 633
G. Albanese, A. Deriu, F. Cavatorta, and A. Rupprecht

The Effect of Intrinsic Curvature on Supercoiling: Predictions of Elastic Theory / 639
I. Tobias and W. K. Olson

Characterization of the Bioactive Form and Molecular Determinants of Recognition of Cyclic Enkephalin Peptides at the δ-Opioid Receptor / 647
C. Chew, H. O. Villar, and G. H. Loew

IR Study of the Proton Acceptor Ability of N-*t*-Butoxycarbonylproline N'-Methylamide / 659
J. Parmentier, K. De Wael, C. Samyn, and Th. Zeegers-Huyskens

Synthesis and Conformational Analysis of N-Glycopeptides. II. CD, Molecular Dynamics, and NMR Spectroscopic Studies on Linear N-Glycopeptides / 665
A. Perczel, E. Kollát, M. Hollósi, and G. D. Fasman

Cyanogen as a Selective Probe for Carbonic Anhydrase Hydrolase Activity / 687
A. A. Karagözler, G. Ghenbot, and R. A. Day

NMR and Computer-Aided Studies of the Three Interchanging Stereoisomers of the Cyclic Hexapeptide *cyclo*[-Pro[1]-Gly[2]-Glu[3](OBzl)-Pro[4]-Phen[5]-Leu[6]-]: Unexpected Observation of a *cis* Isomer of a Secondary Amide Peptide Bond in the Presence of Two *Trans* Proline Peptide Bonds / 693
I. Mc Ewen

Sol–Gel Transition of Alginate Solution by the Addition of Various Divalent Cations: ^{13}C-NMR Spectroscopic Study / 703
Z.-Y. Wang, Q.-Z. Zhang, M. Konno, and S. Saito

Substituent Effects on the Puckering Mode of the Cyclobutane Ring and the Glycosyl Bond of *cis–syn* Photodimers / 713
J.-K. Kim, J. C. Wallace, and J. L. Alderfer

Announcement / 723

Issue 5, May 1993

Lattice Vibrations in Crystalline L-Alanine / 725
D. Durand, M. J. Field, M. Quilichini, and J. C. Smith

Molecular Dynamics of Sickle and Normal Hemogloblins / 735
M. Prabhakaran and M. E. Johnson

Self-Assembly of Bioelastomeric Structures from Solutions: Mean-Field Critical Behavior and Flory–Huggins Free Energy of Interactions / 743
F. Sciortino, K. U. Prasad, D. W. Urry, and M. U. Palma

Heat Capacities of Solid Poly(Amino Acid)s. II. The Remaining Polymers / 753
K. A. Roles, A. Xenopoulos, and B. Wunderlich

A Proton Magnetic Resonance Study of Two Synthetic Agonist–Antagonist Pairs of Bradykinin Analogues / 769
A. Otter, P. Bigler, J. M. Stewart, and G. Kotovych

^{1}H- and ^{13}C-NMR Investigations on *Cis-Trans* Isomerization of Proline Peptide Bonds and Conformation of Aromatic Side Chains in H-Trp-(Pro)$_n$-Tyr-OH Peptides / 781
J. Poznański, A. Ejchart, K. L. Weirzchowski, and M. Ciurak

Differences in Melting Behavior Between Homopolymers and Copolymers of DNA: Role of Nonbonded Forces for GC and the Role of the Hydration Spine and Premelting Transition for AT / 797
Y. Z. Chen and E. W. Prohofsky

Conformational Differences Between Diastereomers of Dnp-Val-Aib-Gly-Leu-pNA Studied by X-Ray Crystal Analyses / 813
T. Yamada, M. Nakao, T. Miyazawa, S. Kuwata, M. Sugiura, Y. In, T. Ishida

Further Characterization of the Kinetic Folding Intermediate of $\alpha\alpha$-Tropomyosin and of Its 142-281 Subsequence / 823
J. Mo, M. E. Holtzer, and A. Holtzer

Unfolding of an α-Helix in Peptide Crystals by Solvation: Conformational Fragility in a Heptapeptide / 827
I. L. Karle, J. L. Flippen-Anderson, K. Uma, and P. Balaram

Probing Protein Structure by Solvent Perturbation of NMR Spectra. II. Determination of Surface and Buried Residues in Homologous Proteins / 839
G. Esposito, A. M. Lesk, H. Molinari, A. Motta, N. Niccolai, and A. Pastore

A Method for Studying the Structure of Uniaxially Aligned Biopolymers Using Solid State ^{15}N-NMR: Application to *Bombyx mori* Silk Fibroin Fibers / 847
L. K. Nicholson, T. Asakura, M. Demura, and T. A. Cross

Announcement / 863

Issue 6, June 1993

Stereochemical Constraints in Peptide Design: Analysis of the Influence of a Disulfide Bridge and an α-Aminoisobutyryl Residue on the Conformation of a Hexapeptide / 865
K. Uma, R. Kishore, and P. Balaram

Carrier Design: Conformational Studies of Amino Acid (X) and Oligopeptide (X-DL-Ala$_m$) Substituted Poly(L-Lysine) / 873
G. Mezö, J. Kajtár, F. Hudecz, and M. Szekerke

Differential Binding of the Enantiomers of Chloroquine and Quinacrine to Polynucleotides: Implications for Stereoselective Metabolism / 887
P. V. Scaria, J. C. Craig, and R. H. Shafer

Elongational Flow Studies on Type IV Collagen: Comparison with Type I / 897
K. Barnard, E. D. T. Atkins, M. A. Taylor, and L. J. Gathercole

A Reexamination of the Conformational Transitions of T4 Thioredoxin / 903
W. Shalongo, M. Jagannadham, and E. Stellwagen

Synthesis, Biological Activity, and Conformational Analysis of [pGlu^6,N-MePhe^8,Aib^9] Substance P(6-11): A Selective Agonist for the NK-3 Receptor / 915
M. Tallon, D. Ron, D. Halle, P. Amodeo, G. Saviano, P. A. Temussi, Z. Selinger, F. Naider, and M. Chorev

Enhanced Solubility of Proteins and Peptides in Nonpolar Solvents Through Hydrophobic Ion Pairing / 927
M. E. Powers, J. Matsuura, J. Brassell, M. C. Manning, and E. Shefter

NMR and Computer-Aided Modeling Studies of the Interactions Between a Cyclic Hexapeptide and the Two Enantiomers of Some Boc- and Fmoc-Amino Acids / 933
I. McEwen

Sequence Dependence of Purine C8H Exchange Kinetics in the Dodecamer 5′-d(CGCGAATTCGCG)-3′ / 943
K. J. Walters and I. M. Russu

On the "Filterable Aggregates and Other Particles" Interpretation of the Extraordinary Regime of Polyelectrolytes / 953
K. S. Schmitz

A Model of the Rabies Virus Glycoprotein Active Site / 961
M. Rustici, L. Bracci, L. Lozzi, P. Neri, A. Santucci, P. Soldani, A. Spreafico, and N. Niccolai

Probing the Influence of Sequence-Dependent Interactions upon α-Helix Stability in Alanine-Based Linear Peptides / 971
S. G. Jacchieri and N. G. J. Richards

Specific Helix Stabilization of Poly(L-Glutamic Acid) in Mixed Counterion Systems / 985
M. Satoh, F. Kato, and J. Komiyama

RESEARCH COMMUNICATION

Evidence for a 3_{10}-Helical Conformation of an Eight-Residue Peptide from ^{1}H-^{1}H Rotating Frame Overhauser Studies / 995
G. Basu and A. Kuki

Issue 7, July 1993

Special Issue: Third Naples Workshop on Conformational Analysis of Peptides: Relationships and Interactions

Editorial / 1001

Improved Molecular Dynamics Simulations for the Determination of Peptide Structures / 1003
D. F. Mierke and H. Kessler

CD of Proline-Rich Polypeptides: Application to the Study of the Repetitive Domain of Maize Glutelin-2 / 1019
F. Rabanal, M. D. Ludevid, M. Pons, and E. Giralt

Effect of Counterion Concentration on the Dielectric Behavior of a Polypeptidic Chain in the Helix–Coil Transition / 1029
F. Bordi, C. Cametti, and G. Paradossi

Noncoded Residues as Building Blocks in the Design of Specific Secondary Structures: Symmetrically Disubstituted Glycines and β-Alanine / 1037
B. Di Blasio, V. Pavone, A. Lombardi, C. Pedone, and E. Benedetti

Crystal State Conformation of Three Azapeptides Containing the AzaProline Residue, A β-Turn Regulator / 1051
A. Lecoq, G. Boussard, M. Marraud, and A. Aubry

Structures of Peptides from α-Amino Acids Methylated at the α-Carbon / 1061
C. Toniolo, M. Crisma, F. Formaggio, G. Valle, G. Cavicchioni, G. Precigoux, A. Aubry, and J. Kamphuis

Conformational and Topographical Considerations in the Design of Biologically Active Peptides / 1073
V. J. Hruby

Bioactive Peptides: Conformational Study of a Cystinyl Cycloheptapeptide in Its Free and Calcium Complexed Forms / 1083
G. Zanotti, A. Maione, F. Rossi, M. Saviano, C. Pedone, and T. Tancredi

Conformational Mobility in Cyclic Oligopeptides / 1093
K. D. Kopple, J. W. Bean, K. K. Bhandary, J. Briand, C. A. D'Ambrosio, and C. E. Peishoff

Crystal Structures of Two Cyclic Pseudopentapeptides Containing $\psi[CH_2S]$ and $\psi[CH_2SO]$ Backbone Surrogates / 1101
S. Ma, J. F. Richardson, and A. F. Spatola

Solid State and Solution Structure of Boc-L-Ala-ΔPhe-ΔPhe-NHMe: A Dehydropeptide Showing Propensity for 3_{10}-Helices of Both Screw Senses / 1111
A. Tuzi, M. R. Ciajolo, G. Guarino, P. A. Temussi, A. Fissi, and O. Pieroni

Conformational Requirements for Molecular Recognition of Acetylcholine Receptor Main Immunogenic Region (MIR) Analogues by Monoclonal anti-MIR Antibody: A Two-Dimensional Nuclear Magnetic Resonance and Molecular Dynamics Approach / 1123
V. Tsikaris, E. Detsikas, M. Sakarellos-Daitsiotis, C. Sakarellos, E. Vatzaki, S. J. Tzartos, M. Marraud, and M. T. Cung

Modifications of the Amide Bond and Conformational Constraints in Pseudopeptide Analogues / 1135
M. Marraud, V. Dupont, V. Grand, S. Zerkout, A. Lecoq, G. Boussard, J. Vidal, A. Collet, and A. Aubry

NMR and Molecular Dynamics Study of Four Carbocyclic Muramyl Dipeptide Analogues / 1149
P. Pristovšek, J. Kidrič, J. Mavri, and D. Hadžl

Issue 8, August 1993

Molecular Dynamics Simulation of the Stability of a 22-Residue α-Helix in Water and 30% Trifluoroethanol / 1159
A. R. Van Buuren, and H. J. C. Berendsen

Conformational Transitions Using Molecular Dynamics with Minimum Biasing / 1167
S. C. Harvey and H. A. Gabb

Synthesis and Conformational Study of Peptides Possessing Helically Arranged Δ ᶻPhe Side Chains / 1173
Y. Inai, T. Ito, T. Hirabayashi, and K. Yokota

Hydrophobicity and Stability for a Family of Model Proteins / 1185
N. Muller

The Contribution of Helical Potential to the In Vitro Receptor Binding Activity of a Neuropeptide Y N-terminal Deletion Fragment / 1195
M. B. Doughty and L. Hu

Crystal Structures of Boc-D-and L-Iva-L-Pro-OBzl: Unturned Conformation of Aib-Pro Sequence Unaffected by Replacement of Me with Et in Aib / 1207
M. Kawai, Y. Omori, H. Yamamura, Y. Butsugan, T. Taga, and Y. Miwa

The Hydration of Proteins in Nearly Anhydrous Organic Solvent Suspensions / 1213
J. H. McMinn, M. J. Sowa, S. B. Charnick, and M. E. Paulaitis

DNA Orientation in Shear Flow / 1225
T. Simonson and M. Kubista

Proton Magnetic Resonance Studies of Bradykinin Antagonists / 1237
X. Liu, J. M. Stewart, L. Gera, and G. Kotovych

Computer Simulations of the Flexibility of a Series of Synthetic Cyclic Peptide Analogues / 1249
A. Thomas, B. Roux, and J. C. Smith

The Loop Problem in Proteins: A Monte Carlo Simulated Annealing Approach / 1271
L. Carlacci and S. W. Englander

The Solution Conformation of Ac–Pen–Arg–Gly–Asp–Cys–OH, a Potent Fibrinogen Receptor Antagonist / 1287
M. J. Bogusky, A. M. Naylor, M. E. Mertzman, S. M. Pitzenberger, R. F. Nutt, S. F. Brady, C. D. Colton, and D. F. Veber

Electromigration Behavior of Poly-(L-Glutamate) Conformers in Concentrated Polyacrylamide Gels / 1299
V. Dolník, M. Novotny, and J. Chmelík

Hybrid Monte Carlo Simulations Theory and Initial Comparison with Molecular Dynamics / 1307
A. Brass, B. J. Pendleton, Y. Chen, and B. Robson

Issue 9, September 1993

Molecular Recognition of Watson–Crick Base-Pair Reversals in Triple-Helix Formation: Use of Nonnatural Oligonucleotide Bases / 1317
V. Mohan, Y.-K. Cheng, G. E. Marlow, and B. M. Pettitt

Individual-Site Binding Data and the Energetics of Protein–DNA Interactions / 1327
H. A. Saroff

Chain Length Dependent Transition of 3_{10}- to α-Helix of Boc-(Ala-Aib)$_n$-OMe / 1337
K. Otoda, Y. Kitagawa, S. Kimura, and Y. Imanishi

Stretching and Overstretching of DNA in Pulsed Field Gel Electrophoresis. I. A Quantitative Study from the Steady State Birefringence Decay / 1347
P. Mayer, J. Sturm, and G. Weill

Stretching and Overstretching of DNA in Pulsed Field Gel Electrophoresis. II. Coupling of Orientation and Transport in Initial Response to the Field / 1359
P. Mayer, J. Sturm, and G. Weill

An NMR and Conformational Investigation of the *trans–syn* Cyclobutane Photodimers of dTpdU / 1365
W. A. Tabaczynski, D. G. E. Lemaire, B. P. Ruzsicska, and J. L. Alderfer

Formation of Several Stable Complexes Between the Minor Components of the Cyclic Tetrapeptide Cyclo-(-Pro[1]-Ala[2]-D-Phe[3]-Leu[4]-) and Some Specific Boc-Amino Acids / 1377
I. McEwen and K. Ottosson

Statistics of RNA Secondary Structures / 1389
W. Fontana, D. A. M. Konings, P. F. Stadler, and P. Schuster

A Formulation for Correlating Properties of Peptides and Its Application to Predicting Human Immunodeficiency Virus Protease-Cleavable Sites in Proteins / 1405
J. J. Chou

Effect of Cationic Drugs on Suprahelical Organization of DNA / 1415
K. G. Krishna, T. K. S. Kumar, and M. W. Pandit

Effect of Various Frictional Models on Long-Time Peptide Dynamics / 1423
K. Kostov, K. F. Freed, and A. Perico

Quinacrine: Spectroscopic Properties and Interactions with Polynucleotides / 1431
S. M. Doglia, B. Albinsson, C. Hiort, B. Nordén, and A. Gräslund

Conformational Analysis of the Type II and Type III Collagen α-1 Chain N-Telopeptides by ^{1}H-NMR Spectroscopy and Restrained Molecular Mechanics Calculations / 1443
A. Otter, P. G. Scott, and G. Kotovych

Secondary Structure of Proteins Associated in Thin Films / 1461
J. Safar, P. P. Roller, G. C. Ruben, D. C. Gajdusek, and C. J. Gibbs, Jr.

RESEARCH COMMUNICATION

Chemo- and Stereoregularity Consecutiveness Governing the Specificity in β-Structure/α-Helix Decision for Solid-State Sequential Hydrophobic Polypeptides Predominant to the Directional Tendency of Individual Amino Acid Residues / 1477
N. Yonezawa, K. Kobayashi, and R. Katakai

Issue 10, October 1993

Molecular Dynamics Simulations of a Winter Flounder "Antifreeze" Polypeptide in Aqueous Solution / 1481
S. M. McDonald, J. W. Brady, and P. Clancy

Photoresponsive Polypeptides: Photochromism and Conformation of Poly(L-Glutamic Acid) Containing Spiropyran Units / 1505
A. Fissi, O. Pieroni, F. Ciardelli, D. Fabbri, G. Ruggeri, and K. Umezawa

Simulation of α-Helix–Coil Transitions in Simplified Polyvaline: Equilibrium Properties and Brownian Dynamics / 1519
W. Schneller and D. L. Weaver

Molecular Dynamics Simulations of Poly(dA) · Poly(dT): Comparisons Between Implicit and Explicit Solvent Representations / 1537
V. Fritsch, G. Ravishanker, D. L. Beveridge, and E. Westhof

On the Interaction of Polypeptides with Bile Salts of Bilirubin-IXα / 1553
M. D'Alagni, A. A. D'Archivio, and E. Giglio

Molecular Dynamics Analysis of a Ribonuclease C-Peptide Analogue / 1567
K. V. Soman, A. Karimi, and D. A. Case

Assessment of Protein Rotational Diffusion by ^{13}C Off-Resonance Rotating Frame Spin–Lattice Relaxation: Effect of Backbone and Side-Chain Internal Motion / 1581
S. X. Wang, A. Stevens, and T. Schleich

Energetics of the Disulfide Bridge: An Ab Initio Study / 1591
W. Qian and S. Krimm

Single-Residue Substitution in Homopolypeptides: Perturbative Helix–Coil Theory at a Single Site / 1605
H. Qian

Structural Versatility of Peptides from $C^{\alpha,\alpha}$-Disubstituted Glycines: Crystal-State Conformational Analysis of Homopeptides from C^{α}-Methyl, C^{α}-Benzylglycine $[(\alpha Me)Phe]_n$ / 1617
G. Valle, M. Pantano, F. Formaggio, M. Crisma, C. Toniolo, G. Precigoux, G. Sulzenbacher, W. H. J. Boesten, Q. B. Broxterman, H. E. Schoemaker, and J. Kamphuis

RESEARCH COMMUNICATIONS

Thermodynamic Analysis "Preferential Solvation" in Protein Solutions / 1627
P. R. Wills and D. J. Winzor

Issue 11, November 1993

Comparative Study of the Interactions of Cisplatin and Carboplatin with Nucleotides Using UV Resonance Raman Spectroscopy / 1631
R. L. Benson and T. L. Gustafson

The Influence of Ionic Strength and pH on the Aggregation Properties of Zinc-Free Insulin Studied by Static and Dynamic Laser Light Scattering / 1643
W. Kadima, L. Øgendal, R. Bauer, N. Kaarsholm, K. Brodersen, J. F. Hansen, and P. Porting

Refined Three-Dimensional Solution Structure of a Snake Cardiotoxin: Analysis of the Side-Chain Organization Suggests the Existence of a Possible Phospholipid Binding Site / 1659
B. Gilqiun, C. Roumestand, S. Zinn-Justin, A. Ménez and F. Toma

Z → B Transition in Poly[d(G-m^{5}C)$_2$] Induced by Interaction with 4',6-Diamidino-2-Phenylindole / 1677
S. K. Kim, S. Eriksson, and B. Nordén

Identification of the Adenine Binding Site in the Ricin Toxin A-Chain by Fluorescence, CD, and Electron Spin Resonance Spectroscopy / 1687
T. S. Ramalingam, P. K. Das, and S. K. Podder

Solid-Phase Synthesis and Stability of Triple-Helical Peptides Incorporating Native Collagen Sequences / 1695
C. G. Fields, C. M. Lovdahl, A. J. Miles, V. L. Matthias Hagen, and G. B. Fields

^{127}I-NMR Studies of Anion Binding to κ-Carrageenan / 1709
W. Zhang and I. Furó

A and Z Canonical Conformations in d(C_nGCG_n) Crystals Characterized by MicroFTIR and MicroRaman Spectroscopies / 1715
H. Sfihi, J. Liquier, L. Urpi, N. Verdaguer, J. A. Subirana, J. Igolen, and E. Taillandier

Dynamics and Structures of DNA: Long-Range Effects of a 16 Base-Pair $(CG)_8$ Sequence on Secondary Structure / 1725
U.-S. Kim, B. S. Fujimoto, C. E. Furlong, J. A. Sundstrom, R. Humbert, D. C. Teller, and J. M. Schurr

Structural Changes in 16S RNA from Escherichia coli upon Unfolding by Urea / 1747
A. A. Timchenko, J. Langowski, and I. N. Serdyuk

Issue 12, December 1993

Intramolecular Interference Effects in Dynamics Light Scattering from Rigid Rings / 1757
J. A. Gebe and J. M. Schurr

Studies of DNA Dumbbells. IV. Preperation and Melting of a DNA Dumbbell with the 16 Base-Pair Sequence $^{5'}$G-T-A-T-C-C-C-T-C-T-G-G-A-T-A-C$^{3'}$ Linked on the Ends by Dodecyl Chains / 1765
M. J. Doktycz, T. M. Paner, and A. S. Benight

Studies of DNA Dumbbells. V. A DNA Triplex Formed Between a 28 Base-Pair DNA Dumbbell Substrate and a 16 Base Linear Single Strand / 1779
T. M. Paner, F. J. Gallo, M. J. Doktycz, and A. S. Benight

Depolarization of Raman Scattering from Some Nucleotides of RNA and DNA / 1791
T. Ueda, K. Ushizawa, and M. Tsuboi

Low Oxygen Affinity Derivatives of Human Hemoglobin by Fixation of Polycarboxylic Dextran to the Oxyform / 1803
F. Prouchayret and E. Dellacherie

A Conformational Study of the Dehydroalanine: Dipeptide and Homopolypeptide / 1811
C. Alemán and J. J. Perez

The Effects of $Cu^{2+}$and Pb^{2+} on the Solution Structure of Calf Thymus DNA: DNA Condensation and Denaturation Studied by Fourier Transform IR Difference Spectroscopy / 1819
H.-A. Tajmir-Riahi, M. Naoui, and R. Ahmad

Overcrossing Spectra of Protein Backbones: Characterization of Three-Dimensional Molecular Shape and Global Structural Homologies / 1829
G. A. Arteca

Biasing a Monte Carlo Chain Growth Method with Ramachandran's Plot: Application to Twenty-L-Alanine / 1843
J. Bascle, T. Garel, H. Orland, and B. Velikson

Self-Consistent Reaction Field Computation of the Reactive Characteristics of DNA Bases in Water / 1851
M. Orozco and F. J. Luque

The Influence of Hydration on the Conformation of Bovine Serum Albumin Studied by Solid-State ^{13}C-NMR Spectroscopy / 1871
R. B. Gregory, M. Gangoda, R. K. Gilpin, and W. Su

Conformation and Interactions of Uteroglobin Fragments 4–14 and 49–65 in Aqueous Solution Containing Surfactant Micelles / 1877
M. Tessari, M. T. Foffani, S. Mammi, and E. Peggion

Quantitative Two-Dimensional NMR Study of Dermenkephalin, A HIghly Potent and Selective δ-Opioid Peptide / 1889
M. Naim, S. Charpentier, P. Nicolas, and D. Baron

Solution Conformation Study of Substance P Methyl Ester and [Nle^{10}]-Neurokinin A (4–10) by NMR Spectroscopy / 1901
M. Zhang and T. C. Wong

Subject Index / 1911

Volume Contents / 1921

Author Index / 1933